New Methods for Monitoring and Modeling Air Quality in Industrial Fence Line Communities

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Current State of Regulatory Air Monitoring

- EGLE air monitoring network is built to analyze regional trends for a small number of chemical species (CO, NO_2, O_3, SO_2, Pb, PM).
- Southeast Michigan has 13 monitoring sites, 7 of which measure ozone.
- One station in Detroit (East 7 Mile) has an automated gas chromatograph system to measure a suite of hydrocarbons every hour.
- Toxics monitoring based on 24-hour sampling with Summa canisters or DNPH cartridges. Many semi-volatile/polar VOCs unsampled.
- Current regulatory approaches can not detect sporadic emission events in fence line communities due to signal dilution by time averaging and distance, limited speciation information, and infrequency of measurements.


TO-Can

Michigan-Ontario Ozone Source Experiment (MOOSE)

- International / intergovernmental collaboration:
  - **United States:** Michigan EGLE, U.S. EPA, NASA, NSF, U.S. Forest Service, U.S. Department of Energy
  - **Canada:** Environment and Climate Change Canada (ECCC), Ontario Ministry of Environment, Conservation, and Parks (MECP)

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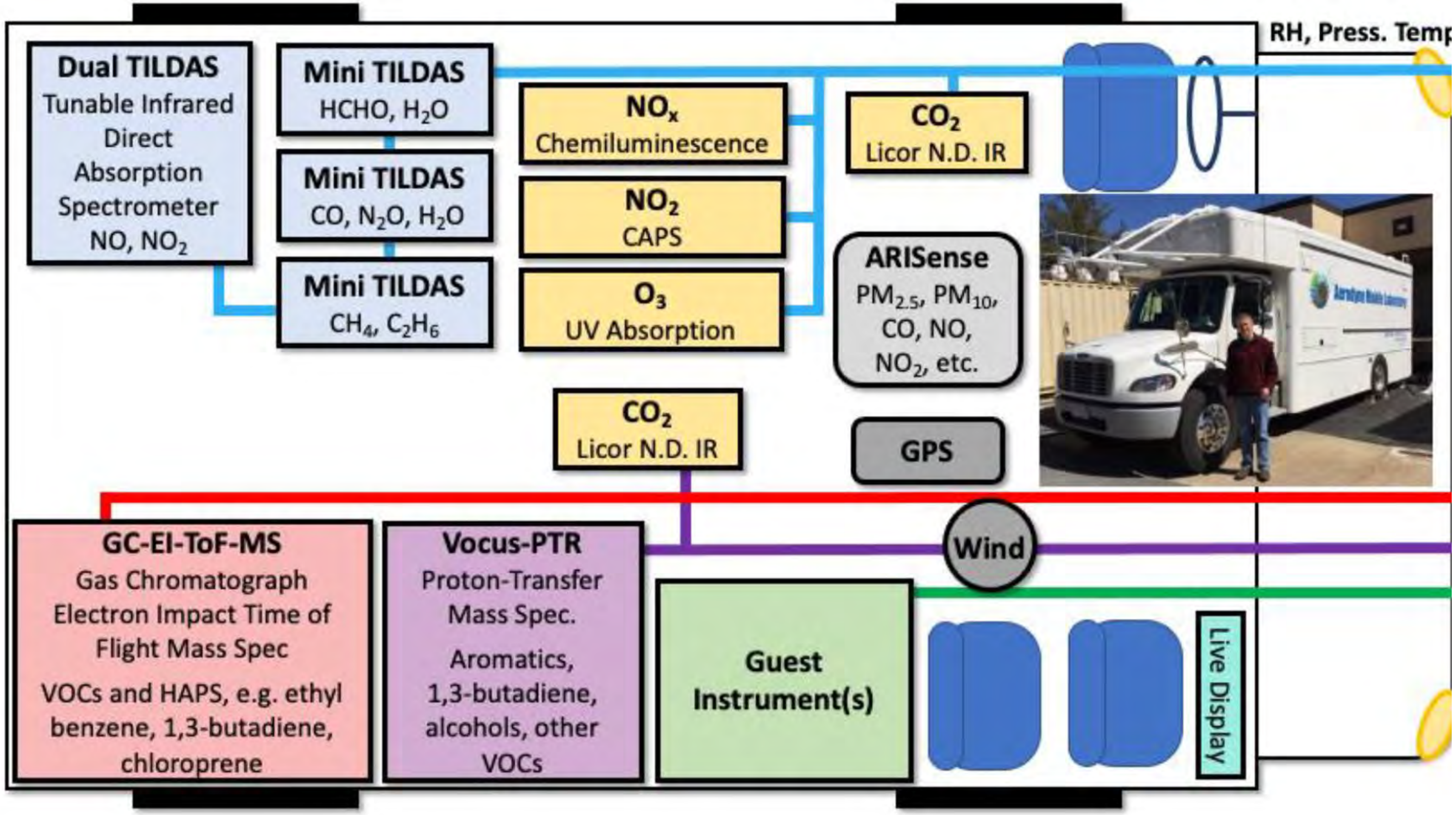
Mobile Real-Time Measurements during MOOSE



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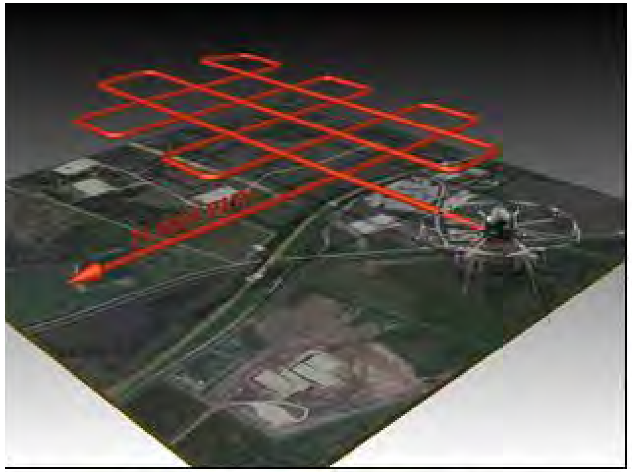
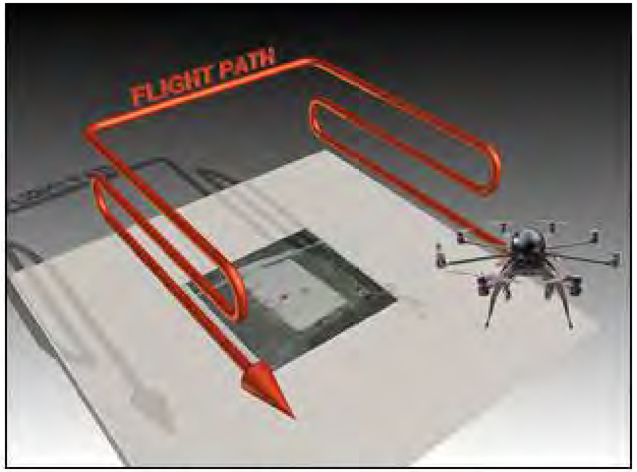
MOOSE Methane Measurements at Landfills

- Two drone measurement platforms:
  - o Aegis IEV2 drone with BlueHalo WP-V2 UAS Weather Payload
  - o DJI M600 heavy-lift drone with a Scentroid DR1000 and a CH_4 Tunable Diode Laser Absorption Spectrometer (TDLAS)
- Supported by two mobile labs (EPA Region 5, University of Michigan) equipped with infrared cavity ringdown spectrometers





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Other Drone Sensors

Chemical Species	Instrument Type	Lower Detection Limit	Resolution	Time Response
Total VOC	Photo-ionization	1 ppb	1 ppb	3 s
Hydrogen Sulfide	Electro-chemical	7 ppb	1 ppb	35 s
Sulfur Dioxide	Electro-chemical	10 ppb	1 ppb	20 s
Formaldehyde	Electro-chemical	10 ppb	10 ppb	60 s
Nitric Oxide	Electro-chemical	10 ppb	1 ppb	60 s

New Approach: Sensor Pods

- Sensor Pod (SPod) technology was developed by the U.S. EPA through its Next Generation Emissions Measurement (NGEM) program.
- SENSIT SPod is a commercial system that contains:
  - a photoionization detector (PID) that measures total VOCs ionizable with a 10.6 eV lamp
  - sensors for measuring wind speed and direction, temperature, relative humidity, and pressure
  - a photo-voltaic power source
  - an onboard operating and data logging system with a secure digital (SD) flash memory card
  - a wireless cell phone modem for remote communication.
- SENSIT SPod can be deployed with a 1.4L evacuated canister grab sample acquisition system. The 30-second grab samples are triggered remotely by an elevated PID signal via a solenoid. Samples are analyzed off-line with Method TO-15.


SENSIT


SENSIT
Technologies

SPods + Sorbent Tubes

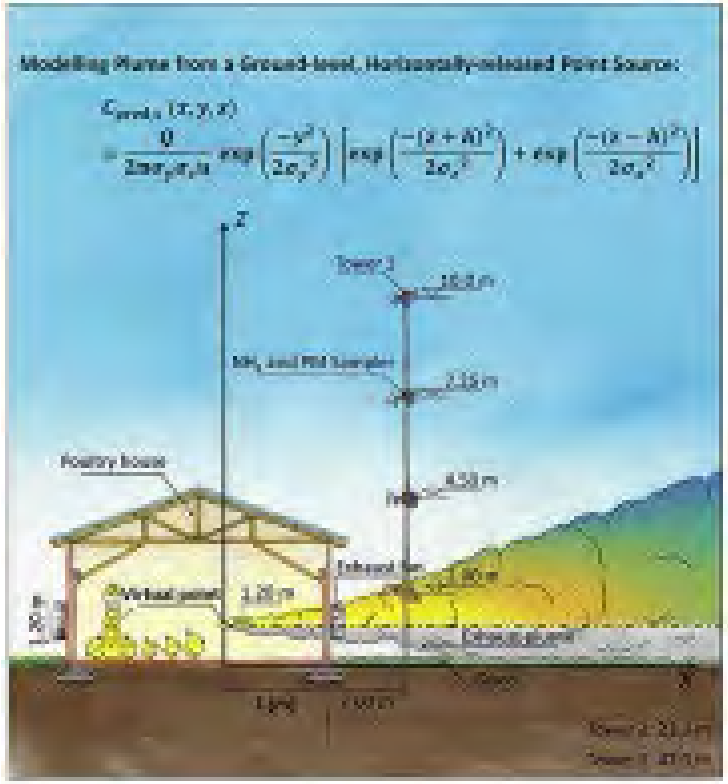
- Proposed monitoring methodology to measure emissions of toxic and odorous VOCs used in automotive paint and coating operations.
- SPods are set up within 500 m of facility fence line to detect emission plumes over a few weeks. The canisters will be triggered whenever the wind blows from the facility toward the neighboring community.
- SPods will be supplemented by 8-hour or 24-hour sampling with sorbent tubes that can be analyzed by Method TO-17. The sorbent tubes will trap many semi-volatile/polar VOCs that escape canister sampling.
- A solvent that can be measured with both TO-15 and TO-17 (e.g., 1,2,4-TMB) will be used as a reference to ratio VOCs measured with TO-17.

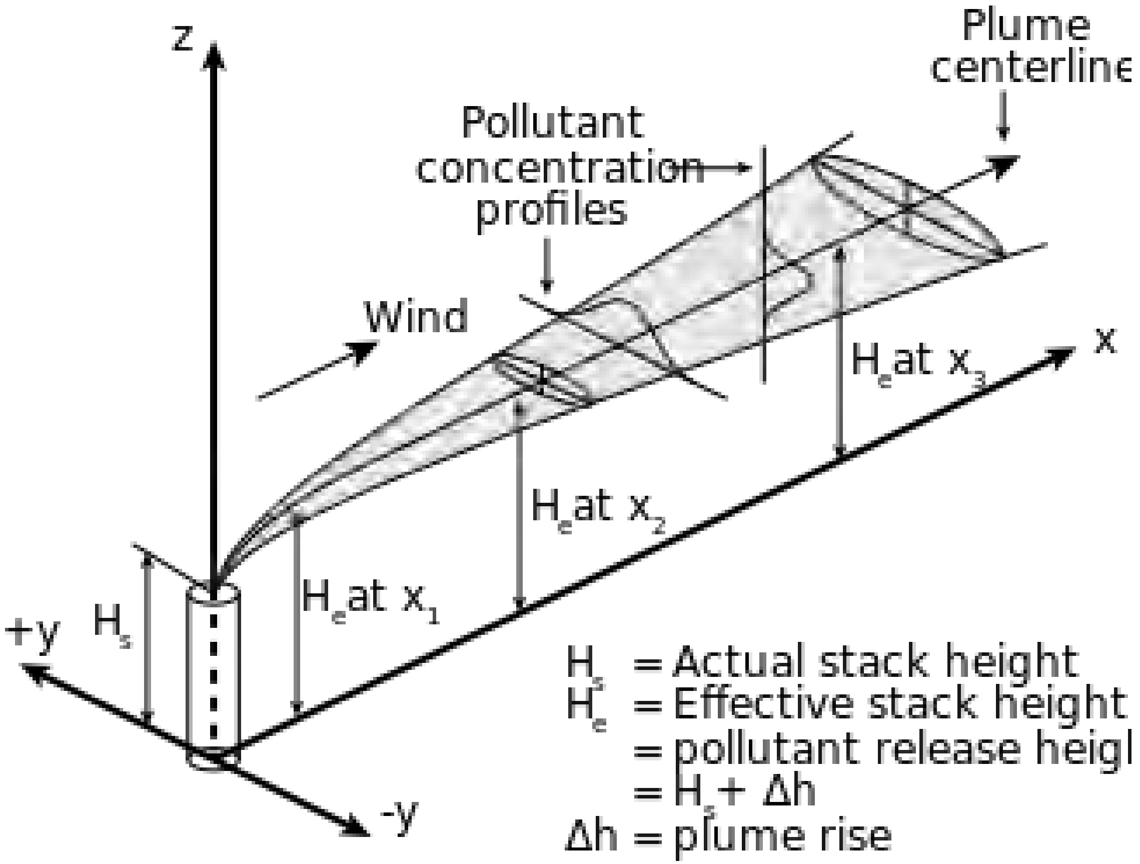
Current State of Regulatory Air Modeling

- AERMOD is a **steady-state Gaussian plume dispersion model** used by EGLE modelers to evaluate air quality permits.

- Regional air quality models (CMAQ, CAMx) are **3-D Eulerian grid models** currently run by LADCO for NAAQS attainment demonstrations in State Implementation Plans.

Gaussian Plume Model





A mathematical formula is applied to a selected number of receptors (locations of human exposure).

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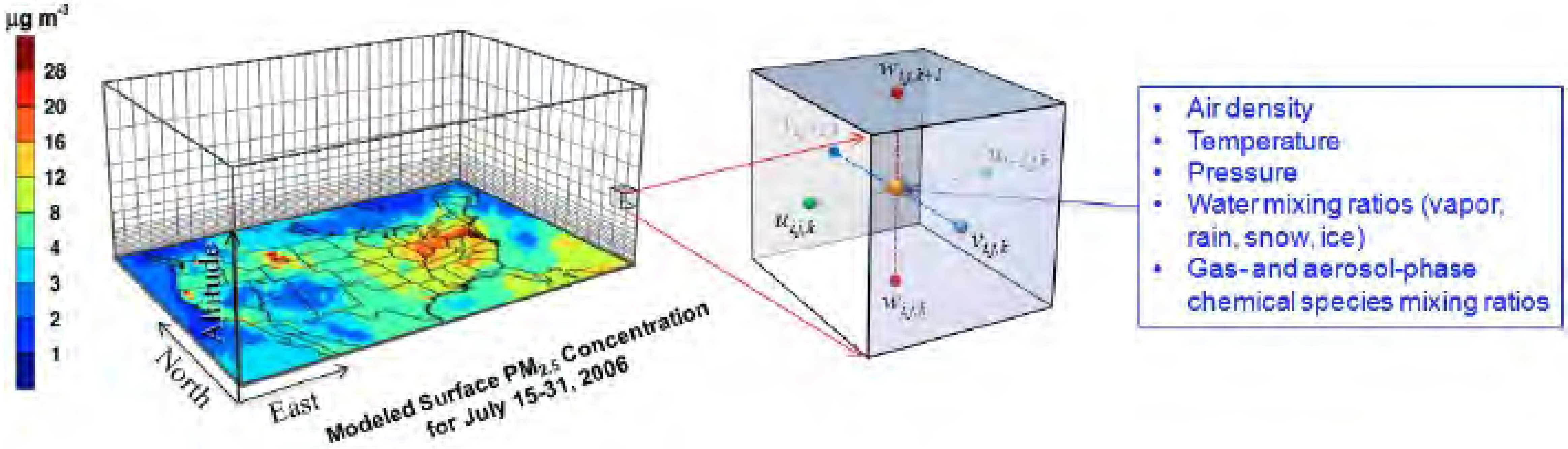
3-D Eulerian Grid Model



The model domain is divided into boxes (grid cells).

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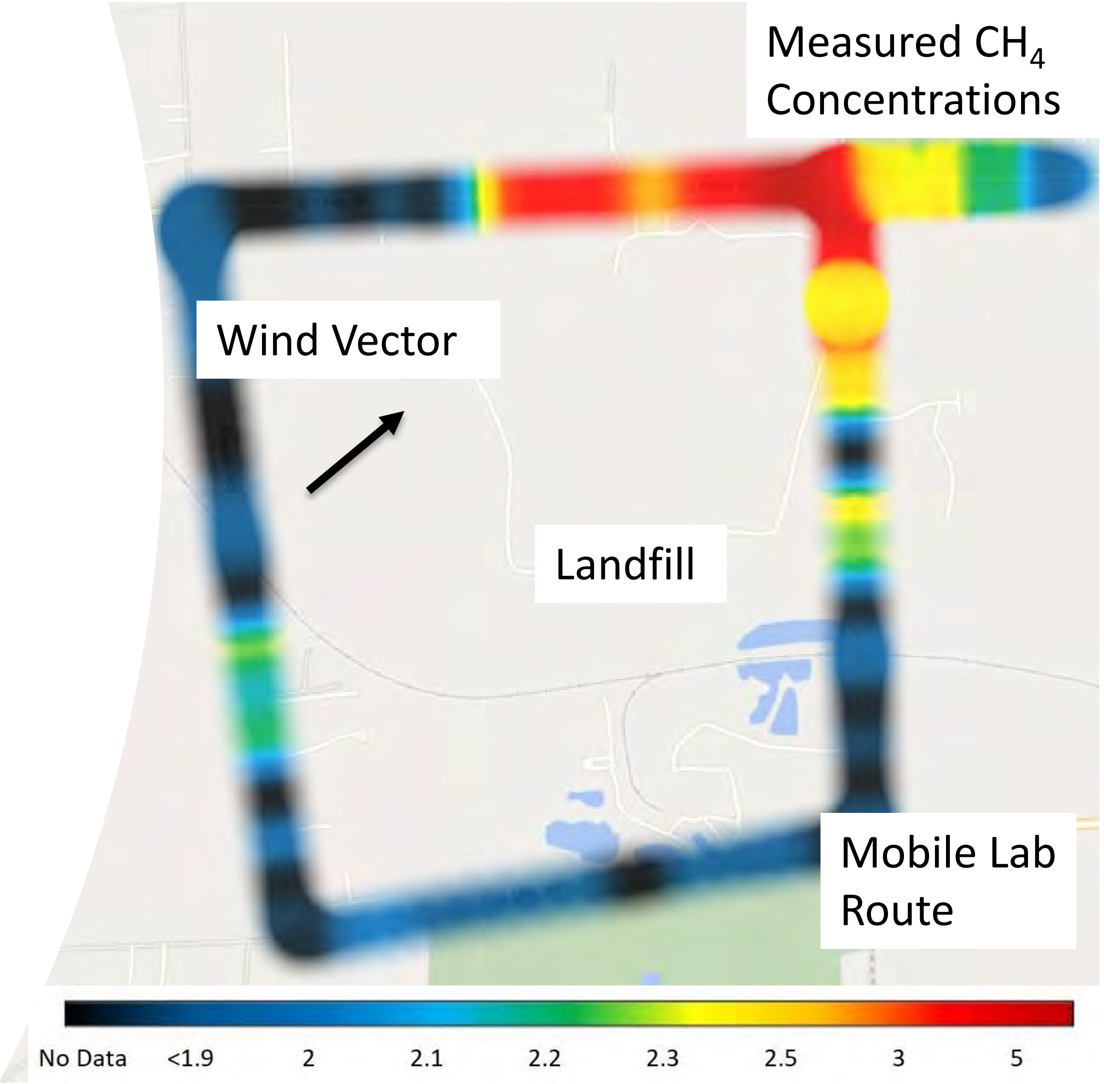
Gaussian Plume Inverse Model

- Permitting applications typically use AERMOD to compute ambient concentrations resulting from reported facility emissions (forward modeling).
- Recoded main aspects of AERMOD, including complex terrain features (e.g., landfills), in the Python language.
- Potential source locations within a landfill were assigned to 100 m × 100 m or 10 m × 10 m horizontal grid cells.
- Inverse model assigned emissions to each landfill grid cell based on ambient air concentration measurements and a multilinear equation solver (optimization problem).

Inverse Modeling Based on Mobile Measurements of Methane

- University of Michigan mobile laboratory measurements performed on June 5, 2021, 10:24 am – 10:39 am.
- Wind speed = 3.1 m/s, wind direction = 246˚
- Pressure = 980 mb, temperature = 299 K
- Convective boundary layer with the following parameters:
  - Roughness length = 0.1 m
  - Cloud cover = 50%
  - Albedo = 0.23
  - Bowen ratio = 0.55
  - Inferred mixing height = 431 m
- Cell resolution: 100 m

Data courtesy of Stuart Batterman



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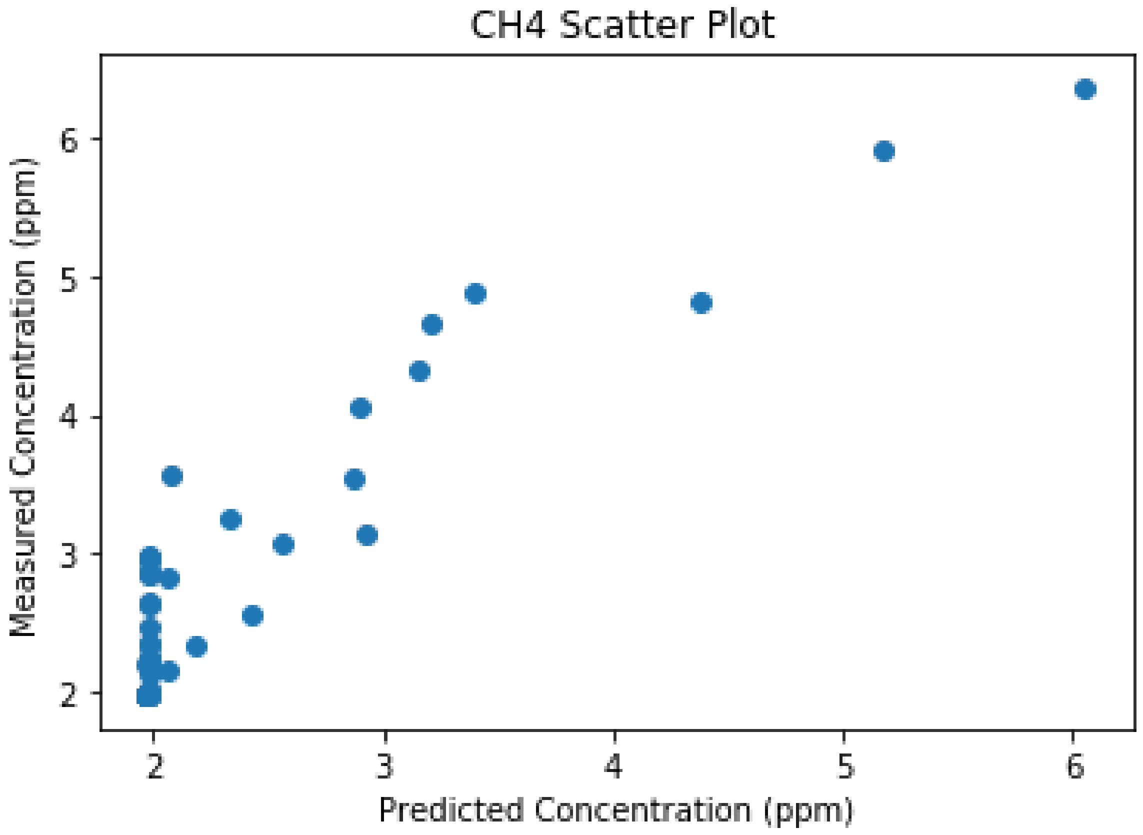
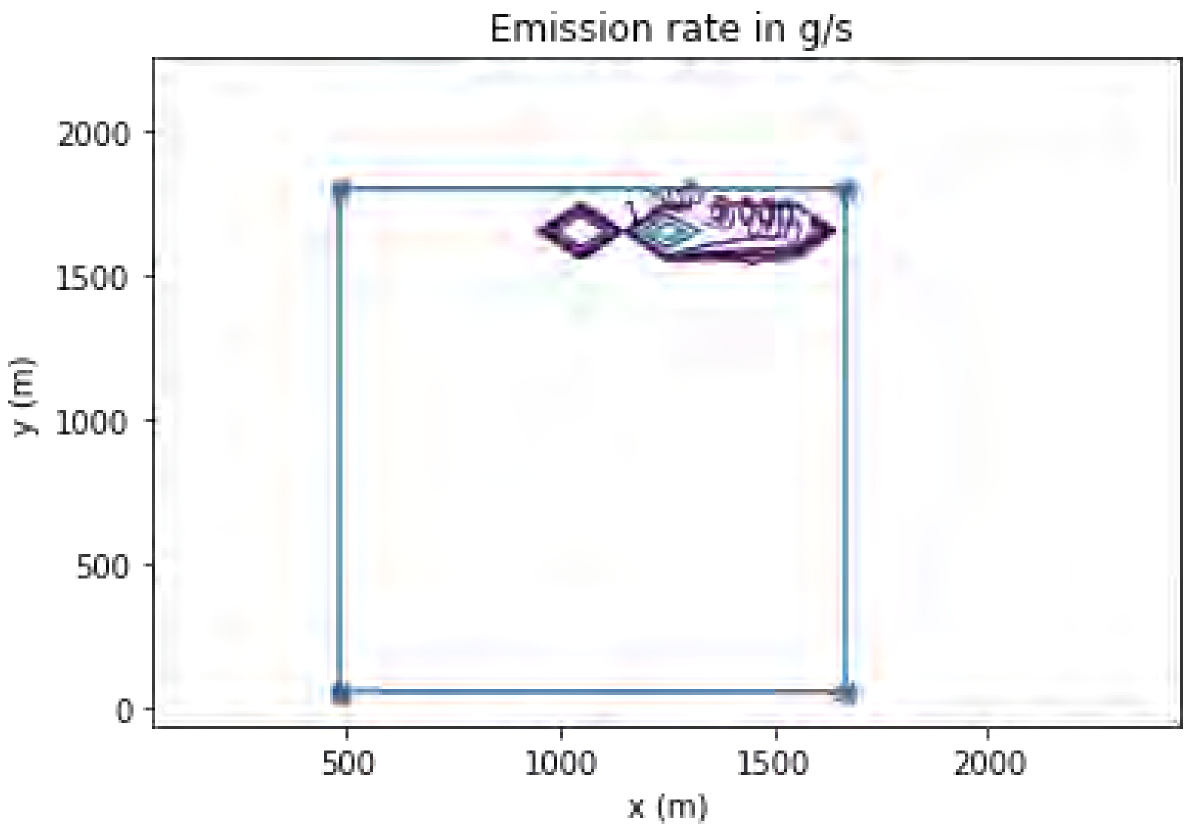
Inverse Model Results





Slope = 1.12, R = 0.905

Total Methane Emissions = 500 kg/h

Note:

In a previous presentation to the Air Advisory Council, the total methane emissions in this case was erroneously reported as 3000 kg/h.

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Microscale Forward and Adjoint Chemical Transport Model (MicroFACT)

- **Fine-scale 3-D Eulerian grid model** **(**400 m horizontal resolution, 10 s time steps) with forward and inverse modes (Olaguer, 2021: *Atmosphere* **12**, 877)
- **Building-sensitive winds** derived from QUIC model
- **Transport** of air pollutants by mean wind (advection) and air turbulence (diffusion)
- **Chemistry** is simulated by 116 gas-phase and 5 heterogeneous reactions
- Can **infer emissions at fine scale** from measurements
- Can simulate **cumulative exposure** to multiple species

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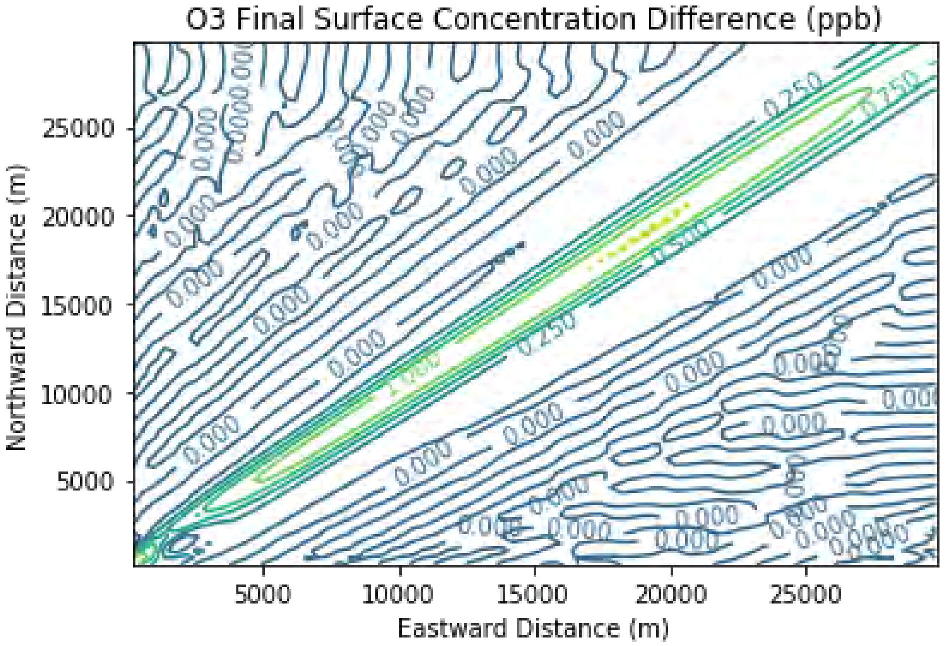
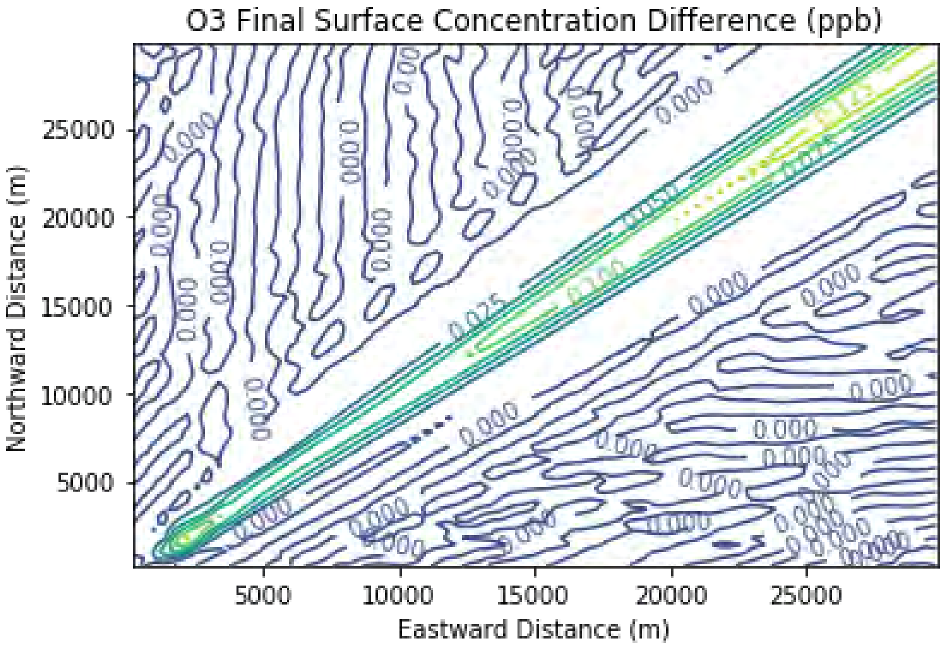
MicroFACT Simulation of Ozone Impact of a Hypothetical Landfill



Additional Ozone over Background due to Combustion Emissions from Flares and Engines

Ozone Enhancement due to Landfill Gas Fugitive Emissions of 3000 $kgCH_4/hr$ Plus Accompanying Organics



Olaguer, E.P. (2021), *Atmosphere 12*, 877. https://doi.org/10.3390/atmos12070877

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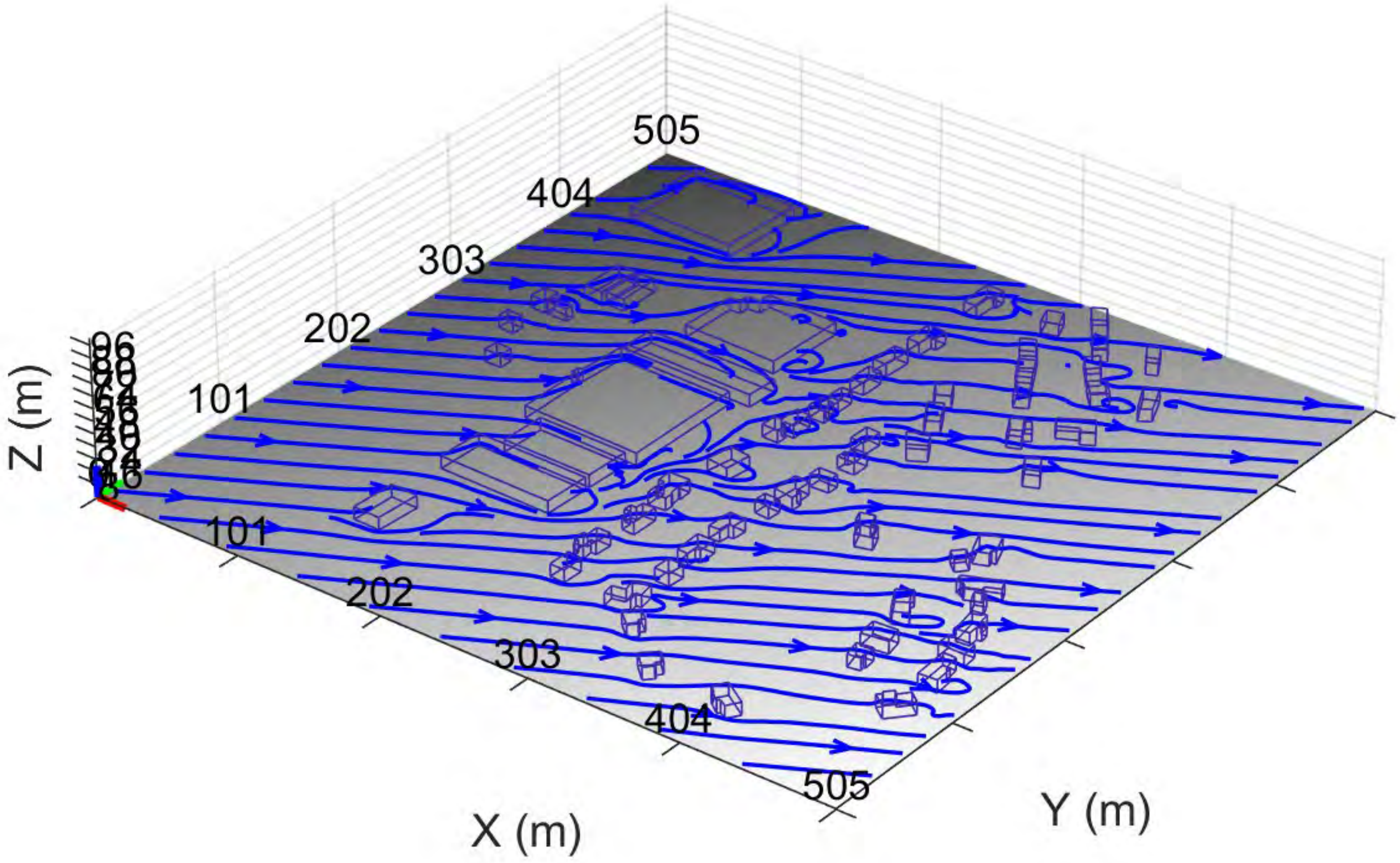
Urban Wind Model



Quick Urban Industrial Complex (QUIC) Model (Los Alamos National Lab)

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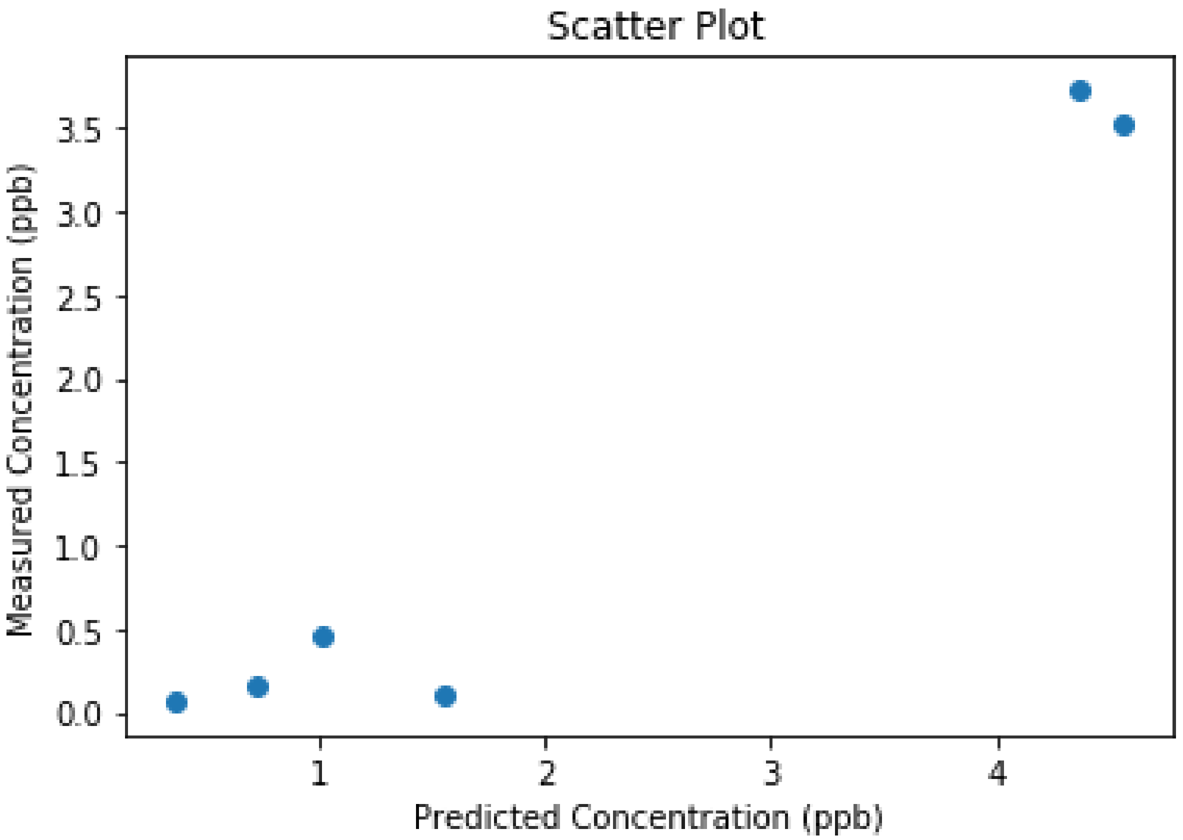
MicroFACT Inverse Modeling of Ethylene Oxide

24-Hour Summa Canister Samples Analyzed by EPA Method TO-15



Inferred Emissions from Medical Sterilization Facility **= 1162 lb/yr**

Slope = 0.926
R = 0.975

Ethylene Oxide Concentrations Predicted by 3D Forward Model based on Emissions Inferred by Inverse Model

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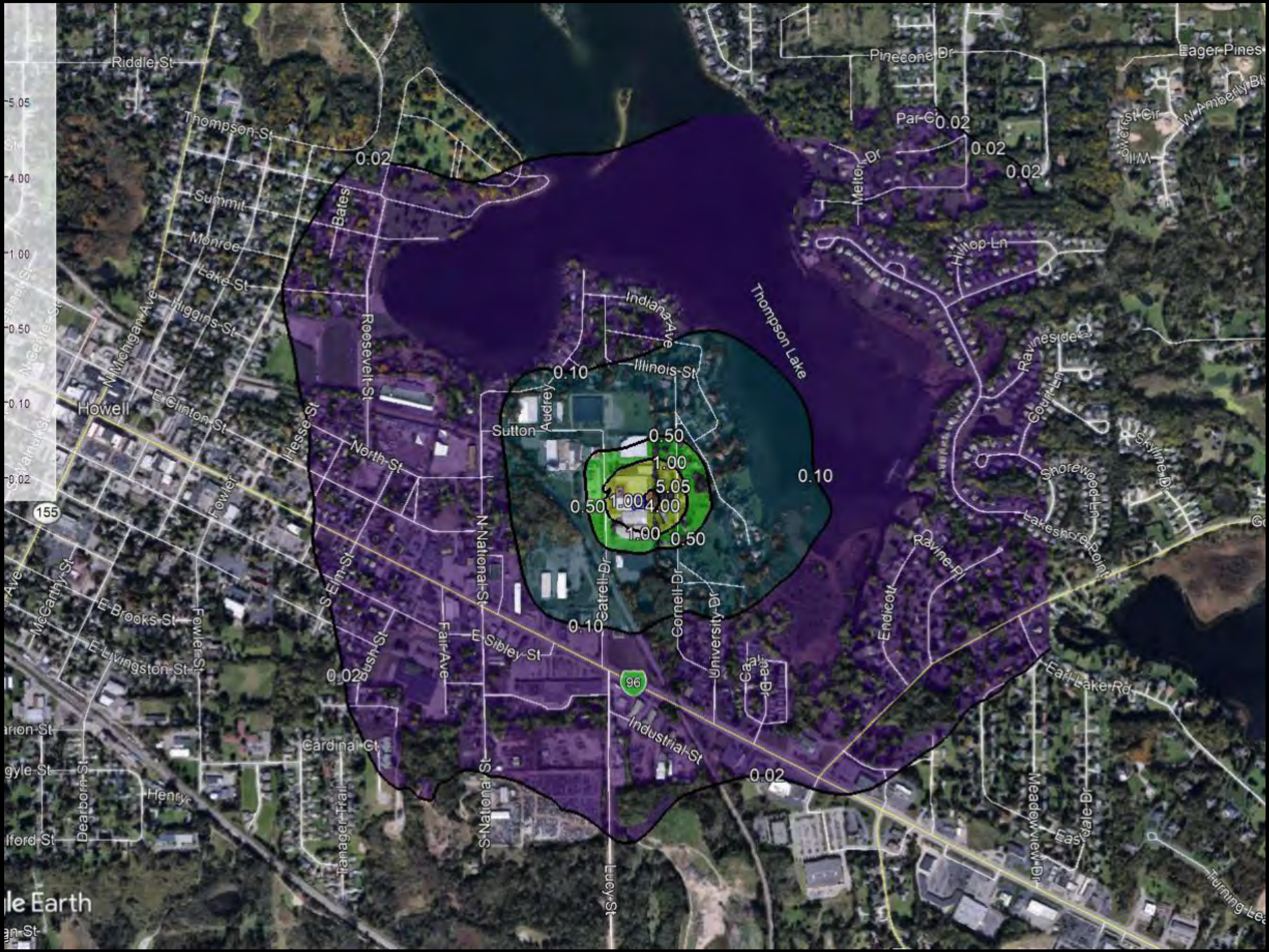

AERMOD Simulation of Annual EtO Impacts Based on Inferred Fugitive Emissions
0.02 ug/m^3 OUTER LIMIT (*Courtesy of Jim Haywood*)

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Key Consideration

- Traditional health risk assessments often rely on measurements of air concentrations as a direct gauge of human exposure.
- Meteorological variability obscures the relationship between episodic concentration measurements and long-term exposure.
- Inverse modeling of emissions based on episodic concentrations provides a better basis of long-term exposure estimates, since emissions don’t depend as much on meteorology.
- Inferred emissions can be fed to AERMOD to estimate long-term exposure and health risk.